DEVELOPMENT OF A GLOBAL QC/QA PROCESSOR FOR OPERATIONAL NOAA 16-18 AND METOP AVHRR SST PRODUCTS

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Abstract

National Oceanic and Atmospheric Administration (NOAA) operational sea surface temperature (SST) products are customarily calibrated and validated (Cal/Val) against *in situ* SSTs from buoy data. However, the match-ups are sparse, geographically biased, and non-uniform in space and time, which complicates their use for continuous, long-term quality control and quality assurance (QC/QA) of the near-real time global satellite-derived SST products. This is best achieved by statistical analysis of anomalies with respect to a global reference SST state. In this study, Bauer-Robinson (1985) SST climatology derived from about 20 years of ground-based observations is used as a reference state.

This work describes the development and initial results of a global near-real time QC/QA processor based on statistical self- and cross-consistency checks. The Global QC/QA Tool (GQT) relies on the analyses of SST anomalies with respect to the reference SST. Anomaly is expected to be distributed normally, although the SST global distribution is highly skewed. The diagnostics are based on the analyses of global histograms of anomalies within a specified time interval (here, 8 days), their four statistical moments (mean, standard deviation, skewness, and kurtosis), and plots of long-term time-series of these statistical parameters. In addition, “artificial trend plots” are used to detect any unrealistic dependencies of SST retrievals upon observational (e.g., latitude, view, or sun angles) or geophysical parameters (e.g., integral water vapor or wind speed). An effort is also made towards identifying extreme outliers (unrealistic retrievals) and their removal from the data.

Initial results using several years of NOAA-16 through 18 and a few months of MetOp-A AVHRR SST products were preliminarily analyzed and inter-compared. Typically, anomaly histograms from different platforms are consistent, with a mean bias of ca. 0.45 K and an RMSD of ca. 1.0 K with respect to Bauer-Robinson 1985 climatological SST. More detailed analyses are underway and their results will be reported elsewhere. In the future, the GQT will also be tested to operationally monitor the quality of SST products from NPOESS/VIIRS and GOES-R/ABI. We emphasize that the GQT is not a substitute for the customary Cal/Val against *in situ* data, rather it is a complementary, near-real time, diagnostic tool for timely detection, diagnosis, and correction of problems in the SST products.

1. INTRODUCTION

Sea surface temperatures (SST) have been operationally retrieved at NESDIS from NOAA AVHRRs, since the early 1980s, using Multi-Channel SST (MCSST) and Non-Linear SST (NLSST) regression algorithms (McClain et al., 1985; Walton, 1988). The SST coefficients are first derived using regression against *in situ* SSTs, early in the satellite mission. SST products are then validated against buoy SST on a monthly basis. This customary validation against *in situ* SSTs proved instrumental in monitoring the quality of satellite SSTs. However, satellite-*in situ* match-ups are sparse, geographically biased, non-uniform in space and time in coverage and quality, and typically available in a substantially delayed mode (c.f., Emery et al., 2001; O’Carroll et al., 2006). “Validation” of SST products against other global reference fields (referred to here as the “global QC/QA”) is thus needed.

This can be realized by analysis of anomalies in satellite SST with respect to either ground-based (e.g., Bauer-Robinson 1985) or satellite (Pathfinder AVHRR SST, Kilpatrick et al., 2001) climatologies, or from blended satellite/*in situ* data, e.g., Reynolds-Smith v2 (Reynolds et al., 2002).

This work describes the development and preliminary results of a statistical global QC/QA tool (GQT), drawing upon some previous pilot studies (e.g., Ignatov et al., 2004). The GQT is based on the analysis of SST anomalies with respect to available reference states (satellite SST – reference SST) on a global scale, assuming that the global anomaly is distributed quasi-normally. The statistical parameters of the Gaussian distribution, along with a multitude of other monitoring tests, can be used as SST quality indicators and for cross-platform product comparisons.

Statistical analyses are performed with both pixel level and gridded level data. At the pixel level, diagnostics are based on the analyses of anomaly histograms and time series of their first four statistical moments (mean, standard deviation, skewness, and kurtosis). The key element of the pixel level analyses is identification and removal of outliers from the data, which would otherwise corrupt the gridded products analyzed in the second stage. The current technique detects outliers based on "mean $\pm$ 4 $\times$ standard deviation" criterion. Improvement to this outlier detection is currently being explored. Grid level analyses are comprised of trend-plots (mean and RMSD anomaly vs. correlated variables, such as latitude, view, or sun angle etc.) and global anomaly maps.

The GQT is designed for constant monitoring of the SST products, in near-real time (daily to weekly time scale), to identify and diagnose problems (e.g., sensor malfunction, residual cloud, or deficiency in retrieval algorithms). Codes to perform specific tasks are designed in Interactive Data Language (IDL) and the implementation is largely automated for uninterrupted QC/QA of the products. A brief description of the data from the NOAA heritage Main Unit Task (MUT) SST orbital processor, used for GQT demonstration, is presented in the next section. Preliminary results and analysis for pixel level and grid level are discussed in sections 3 and 4, respectively. Conclusions and plans for future improvements are given in section 5.

2. SST DATA AND OTHER INFORMATION USED IN THE STUDY

In this study, SST products from the NOAA Main Unit Task (MUT) heritage SST orbital processor (McClain et al., 1985; McClain, 1989; Walton, 1988) are used. The MUT system ingests AVHRR 4 km global area coverage (GAC) data, performs calibration and navigation, and generates top-of-atmosphere brightness temperatures (BT) with an effective spatial resolution of ~8 km for resulting pixels. Subsequently, applying day and night SST algorithms, SST retrievals are generated and stored as satellite-specific rotation files containing retrievals from the last 8 days (referred to as SSTOBS file). Related information is also appended to each of the retrievals, i.e., time, latitude, longitude, satellite zenith angle (SZA), sun angle, day/night flag, azimuth angle, reflectance in the solar reflectance bands, BT in the thermal emission bands, and the nearest Bauer-Robinson 1985 climatological SST. The retrievals are restricted to SZA < $\pm$53°. A summary of MUT products is given by Ignatov et al., 2004. In this work, NOAA 16-18 and MetOp-A MUT SST observation data were analyzed for the following time periods: NOAA-16, 17 from 13 July 2004, NOAA-18 from 16 August 2005, and MetOp-A from 2 April 2007 through 22 August 2007.

3. GQT PROCESSING OF PIXEL LEVEL ANOMALY

In the pixel level GQT processing, MUT SST anomalies are read in and their global histograms are generated separately for day and night data for the SSTOBS file being processed. The first four parameters (mean, standard deviation, skewness, and kurtosis), number of global retrievals, and outlier summary information are annotated on the histograms. These data are also stored in a tabulated form for subsequent generation of time-series plots.

3.1. Histograms of global SST anomalies

Figure 1 shows typical histograms of anomalies for MetOp-A AVHRR SST for the period from 13 August 2007 to 22 August, 2007 (top panel: day, bottom panel: night). The statistical parameters are annotated on the histograms. Typical mean anomaly is ~0.45 K and typical RMSD (Stdv) is ~1 K with respect to Bauer-Robinson climatological SST. Daytime SST shows more variability than nighttime SST. Such histograms are generated for SST products from all available platforms and are animated for visualization and monitoring purposes.

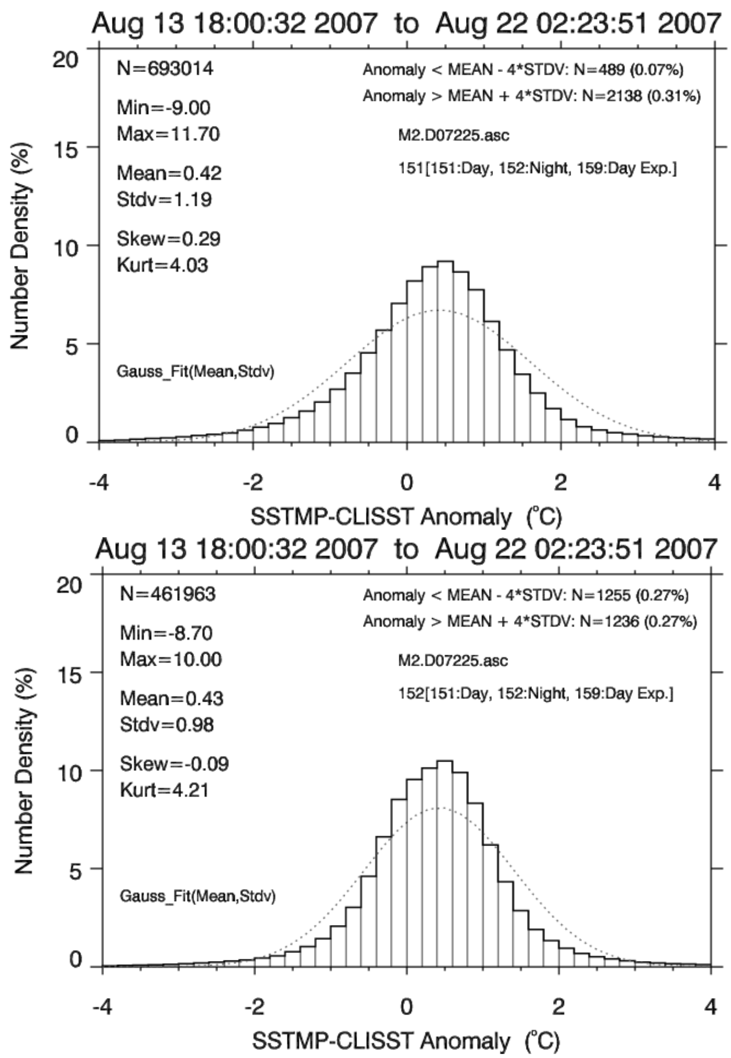

Figure 1: **Histograms of global anomalies (MetOp-A SST – Bauer-Robinson, 1985). Number of observations, minimum, maximum, mean, standard deviation, skewness, and kurtosis of anomalies are annotated and Gaussian fits using sample mean and standard deviation are shown. The number of low and high outliers are shown on top right (top panel: day, bottom panel: night).**

3.2. Time-series plot of global statistical moments

Figure 2 shows time series of global number of observations, mean, standard deviation, skewness, and kurtosis of SST anomalies for NOAA 16-18 and MetOp-A (left panel: day, right panel: night). Each point represents an 8 day period of global statistics. Mean anomalies from N17 and N18 during nighttime are highly consistent, whereas N16 shows anomalous behavior due to sensor problems (Figure 2b).

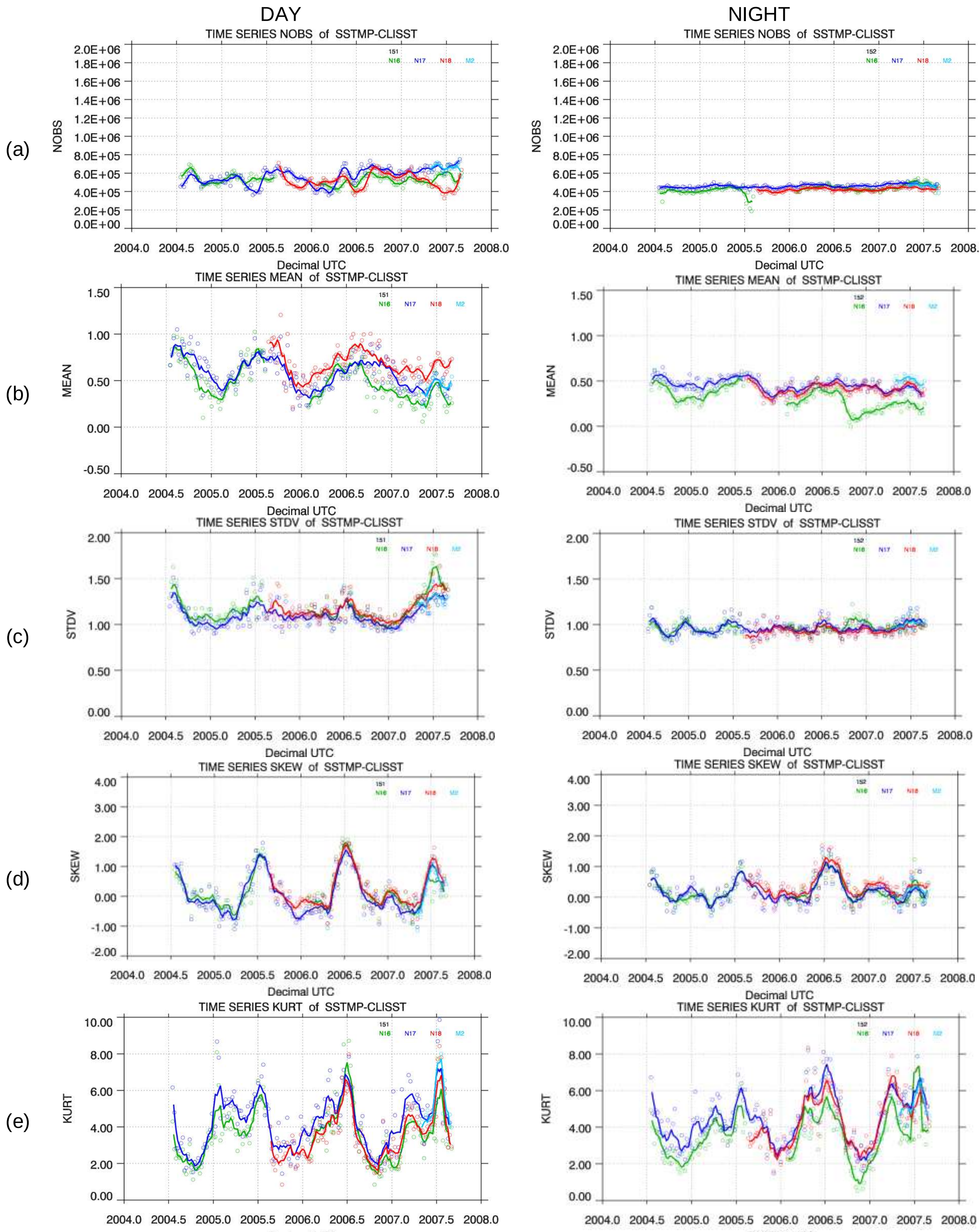

Figure 2: **Time series of global (a) number of observations, (b) mean, (c) standard deviation, (d) skewness, and (e) kurtosis of anomalies (satellite SST – expected state SST) for 4 platforms depicted in different colors: N16: NOAA-16 (green); N17: NOAA-17 (deep blue); N18: NOAA-18 (red); M2: MetOp-A (light blue). Left panel: day, right panel: night. Each point represents 8 days of global data (NOBS~ 500,000).**

Typically, Stdv (Figure 2c) is 0.9-1.1 K during night and 1-1.5 K during day (*c.f.* 0.5 K RMSD typical of global validation against *in situ* data). Higher order moments (skewness, kurtosis) should be zero for a perfect Gaussian distribution. Larger skewness or kurtosis may indicate either increased errors in the product or in the reference state, and can also be further interpreted in terms of root causes (e.g., residual cloud). Using a different reference state may result in a different set of statistics. However, this is not expected to affect the cross-platform (in)consistency. In the newer AVHRR Clear-Sky Processor for Oceans (ACSPO), currently being developed at NOAA NESDIS, multiple reference SSTs (e.g., Reynolds and NCEP RTG SSTs, Pathfinder SST) will be available for GQT analyses.

4. GRIDDING AND ANALYSIS OF GLOBAL ANOMALY MAPS AND TREND-PLOTS

For grid level analysis, first the SST anomalies (satellite – reference) are calculated and then local time, scattering angle, and glint angle are determined, for a given SSTOBS file. Once the anomalies and extra information are known, all the variables are sampled to 1°×1°×24h grid cells (flexible parameter in GQT) and the gridded data are written to a newly created GRDOBS file. Gridding is based on simple averaging, i.e., sum of a variable within a Lat×Lon×24h cell divided by the number of observations (NOBS) in that cell. The NOBS is also stored for each grid-cell, which may serve as a proxy (inverse) for ambient cloud amount. The gridding procedure also has the flexibility for the user to choose whether “outliers” are to be removed or retained at the pixel level.

Figure 3 shows global maps of MetOp-A SST anomalies w.r.t. Bauer-Robinson 1985 climatology.

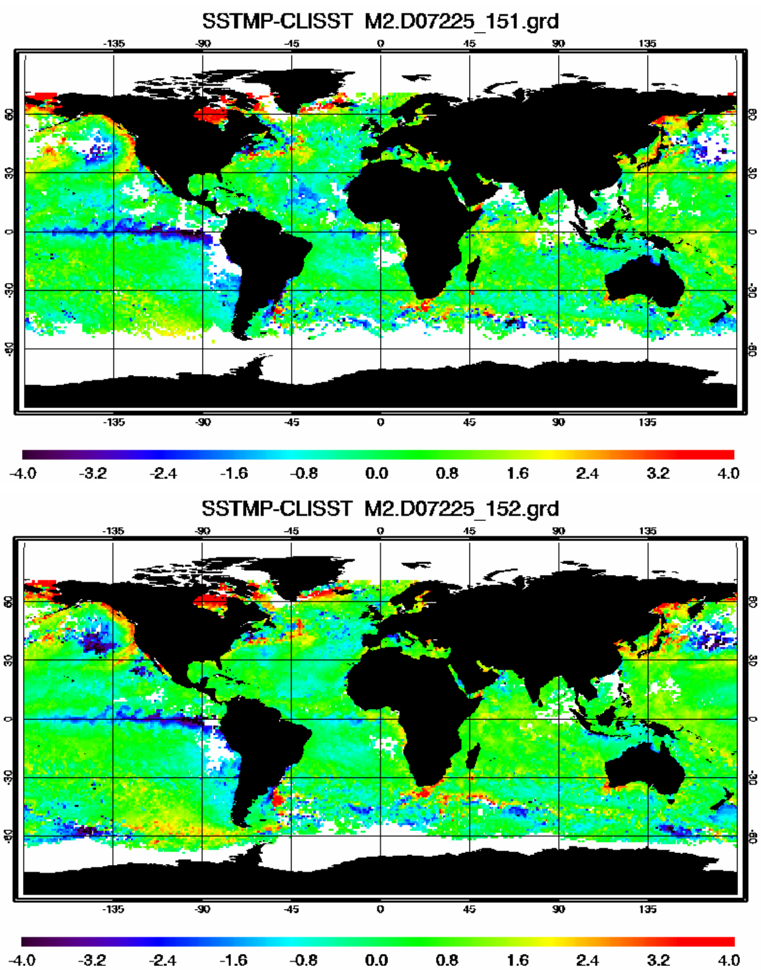

Figure 3: **Global SST anomaly (with respect to Bauer-Robinson 1985) maps from MetOp-A AVHRR for 8-days’ data from 13 August to 22 August, 2007 (top-panel: day, bottom-panel: night).**

The data are for 13 August to 22 August 2007 and outliers were removed at the pixel level using "mean $\pm 4 \times$ Stdv" screening. Time series of bias maps are also animated (not shown) for easy visual separation of "signal" from "noise" in monitoring seasonal geographical variations of global SST anomalies.

In this study, "trend-plot" is defined as a plot of anomalies as functions of correlating observational or geophysical variables, e.g., anomaly as a function of SZA, column water vapor etc. Figure 4 shows MetOp-A SST anomalies as a function of SZA.

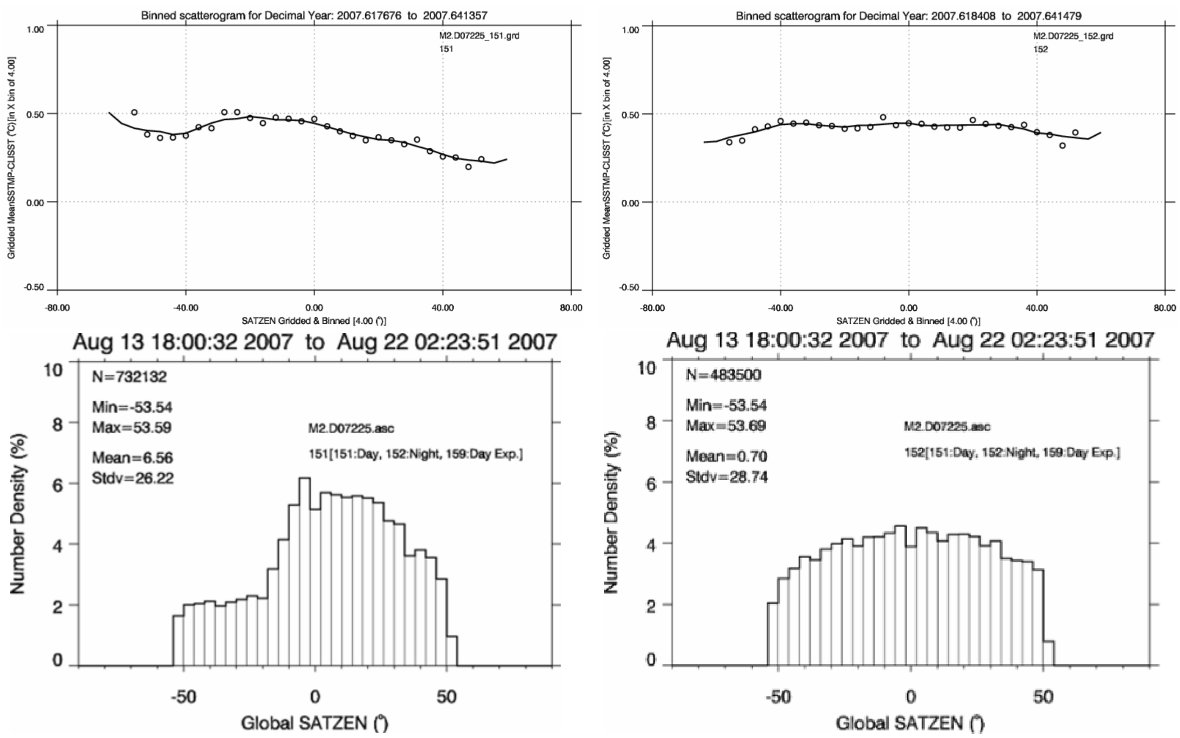

Figure 4: **Trend in the mean gridded SST anomalies as a function of satellite zenith angle (SZA) for MetOp-A AVHRR 8-days' data from 13 August to 22 August, 2007 (left panel: day, right panel: night). Anomalies are averaged within each 4° SZA bin. Corresponding global frequency distributions for day and night SZA are shown below the trend plots to show statistically significant ranges of SZA.**

Note that similar "trend plots" are also generated as a function of other observational (e.g. solar zenith angle, number of points in a grid etc.) and geophysical parameters (water vapor, wind speed) and are animated. All of these trend plots facilitate detection of algorithm/sensor malfunctions and assessment of performance of the SST products throughout their lifetimes.

SUMMARY AND OUTLOOK

Customarily, SST products are validated against *in situ* SST measured by buoys. Match-ups are geographically biased, sparse and require a long time to accumulate sufficient statistics which complicates their use for near-real time QC/QA. A global QC/QA tool (GQT) was developed for statistical comparison of SST products against global reference SST fields and tested with multi-platform SST products derived at NESDIS using the Main Unit Task (MUT) heritage orbital processor. Bauer-Robinson (1985) SST climatology was used as a reference state.

The SST anomaly (satellite SST – climate SST) histograms show exemplary cross-platform consistency, with a mean bias of ca. 0.45 K and an RMSD of ca. 1.0 K. The time-series of the number of observations, mean anomaly, and its standard deviation, skewness, and kurtosis from different platforms closely resemble each other and show similar seasonal variations. If another reference state is chosen, absolute value of the four statistics may change, but this is not expected to affect their cross-platform consistency. Trend plots from gridded anomaly were shown for demonstration purposes, which are being operationally used for timely identification of unwanted dependencies in the SST products due to SST algorithm, cloud screening, or sensor performance.

The GQT facilitates routine monitoring of SST products, in a near-real time. Upon successful testing with the new MetOp SST processor ACSPO, which is currently being developed at NESDIS, the GQT will also be implemented to operationally monitor the quality of SST products derived from other sensors and platforms, e.g., NPOESS/VIIRS and GOES-R/ABI SST products. The same tool may also be used for statistical analysis of other products, e.g., aerosols, land surface temperature, etc. and for validation of radiative transfer models.

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